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To: [Eric Blischke/R10/USEPA/US@EPA](#)
Subject: Food Web Model Comments
Date: 06/09/2008 12:05 PM
Attachments: [Round 2 Report AppendixEComments.doc](#)

Hi Eric,

Here are the comments I started on the food web model. I didn't get to finish them, but I have added some here that area important in regards to how water concentration is handled. Basically, my comments boiled down are:

- 1). Revert back to the uncalibrated Gobas model. We should be looking critically at fine tuning values to get agreement - use hypothesis testing to test the science. You aren't always sure the data you are using for calibrating is correct either. Instead, hypothesis test by comparing the concentration measurements of the same species between observed and predicted. This lets you test how well you model works.
- 2). Building off what is stated in (2), using model performance analysis as outlined by Gobas, which evaluates the ratio of predicted and observed concentrations. Ideally it would be 1 (no model bias), but we should be relying on observed versus predicted to give an estimate of uncertainty. This is something the LWG model does not do because of its over calibration. Let the data show you how uncertain the model is. This is different that model uncertainty analysis, which should be avoided because many parameters are correlated. It is therefore difficult to apply Monte Carlo simulations of uncertainty. The only parameters that are NOT correlated and a true uncertainty analysis could be performed would be lipid content, temperature, and Kow.
- 3). Evaluate empirical data (forward calculation) critically (as stated in 1 and 2) before we jump into the back calculation of PRG development. We should all agree on the "model" used for the back calculation.
- 4). I think there is going to be a lot of discussion regarding contributions between water and sediment to fish tissue. I think the appropriate place to do this is with the empirical data before the backcalculation. As Carl said, there are multiple possibilities in achieving acceptable fish tissue concentrations with the back calculation. However, it is more defensible to deal with this question with the empirical data. This will entail a discussion on how water is handled in the model, something that both Bruce and I have commented on in previous versions. Basically, total water concentrations overestimates fugacity in water (tendency of contaminant in water to partition to fish tissue). This is esp. true where there is a lot of TSS or particulate organic matter in the water. The chemical will be bound up on particulates and not very available to the fish. To get around this, you can use truly dissolved measurements from the field so this overestimate does not occur. This was the comment on a previous version, but instead they used a generic equation to go from total to dissolved. If this is done wrong, the model may show more may be coming from water then is reality - underestimating the contribution from sediment. And trust me, more is coming from the dietary pathway and sediment based on fugacity. I would need a few minutes and some pictures to show you why. This comment is not in my main comment yet - I didn't get to it.

As a side note, I asked Gobas what he would definitely collect data on (and be careful of) - his response was:

- Conc.. of organic carbon in the water phase (this helps with #4) and a very important one for catching disequilibrium - a large factor in chemical movement in the environment.
- Lipid Contents
- Sediment / Water disequilibrium (also related to above) - this controls the relative uptake of chemicals in the water versus the diet
- Use sediment conc.. in the top 1 cm to 1/2 cm (most bioavailability)
- Use data on PCB congeners only

-****Percentage of overlying water is a "tricky" one to get right. Important for those that bury into sediment because fraction of pore water ventilated by these organisms is at a higher fugacity than overlying water. However, this is a sensitive parameter and should be changed with care (I don't think we have better info and should stick with Gobas parameters).

More than you wanted, but maybe we could talk soon about this. I would like to actually go over the Gobas stuff with you if you have the time and the inclination. I haven't looked at the comments from Larry Burkhard. I will take a look and see if we had similar comments.

-Jennifer